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chain nodes :

10 11 12 13 14 15 16 23

ring nodes :

1 2 3 4 5 6 7 8 9 17 18 19 20 21 22

chain bonds :

2-15 7-10 10-11 11-12 12-13 12-14 15-16 16-22 21-23

ring bonds :

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exact/norm bonds :

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exact bonds :

7-10 10-11 11-12 12-13 12-14

normalized bonds :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:CLASS

L1 STRUCTURE UPLOADED

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100.0% PROCESSED 25 ITERATIONS 0 ANSWERS SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE** BATCH **COMPLETE**

800 PROJECTED ITERATIONS: 200 TO PROJECTED ANSWERS: 0 TO

0 SEA SSS SAM L1

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L3 1 SEA SSS FUL L1

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L3 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN

RN 844831-94-3 REGISTRY

Entered STN: 10 Mar 2005

CN Benzenesulfonamide, N-[1-[2-(dimethylamino)ethyl]-1H-indol-5-yl]-2-nitro-(CA INDEX NAME)

C18 H20 N4 O4 S

MF SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE) 3 REFERENCES IN FILE CAPLUS (1907 TO DATE) => file caplus COST IN U.S. DOLLARS

SINCE FILE TOTAL. ENTRY SESSION 180.82 181.03

FULL ESTIMATED COST

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3 L3 L4

=> d ibib abs hitstr 1-3

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:136598 CAPLUS

DOCUMENT NUMBER: 142:240323

TITLE: Active substance combination comprising a compound with NPY receptor affinity and a compound with 5-HT6

receptor affinity

INVENTOR(S): Torrens Jover, Antoni; Mas Prio, Josep; Dordal Zueras,

Alberto; Codony Soler, Xavier; Merce Vidal, Ramon; Aurelio Castrillo Perez, Jose; Frigola Constansa,

Jordi; Buschmann, Helmut-Heinrich Laboratorios del Esteve S. A., Spain

PATENT ASSIGNEE(S):

SOURCE: PCT Int. Appl., 427 pp. CODEN: PIXXD2

DOCUMENT TYPE: Pat.ent. LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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PRIORITY APPLN. INFO.:
                                           ES 2003-1815
                                                               A 20030730
                                           WO 2004-EP8514
                                                               W 20040729
OTHER SOURCE(S):
                      CASREACT 142:240323; MARPAT 142:240323
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- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- AB The present invention relates to an active substance combination comprising at least one compound I (R1-R4 = H, halo, alkyl, etc.; R5 = H, alkyl, (un)saturated cycloalkyl; R6-R9 = H, alkyl, (un)saturated cycloalkyl, etc.;
 - A = CHR18, CHR18CH2; B = alkyl, (un)saturated cycloalkyl, etc.; R10 = H, alkyl, (un)saturated cycloalkyl, etc.; R11 = alkyl, (un)saturated cycloalkyl, etc.; NR10R11 = (un)saturated heterocycly1; R18 = H, alkyl, (un)saturated cycloalkyl, etc.] with neuropeptide Y-receptor affinity, preferably neuropeptide Y5-receptor affinity, and at least one compound with 5-HT6 receptor affinity (such as II [R1 = H, alkyl, Ph, CH2PH; R2 = NR4R5, (un)saturated (hetero)cycloalkyl, etc.; R3 = H, alkyl; R4, R5 = H, alkyl; or NR4R5 = (un)saturated heterocyclyl; A = (un)substituted (hetero)aryl; n = 0-4]), a medicament comprising said active substance combination, and the use of said active substance combination for the manufacture of a medicament. Synthesis of amides I and sulfonamides such as II is described in examples. E.g., a multi-step synthesis of III.HCl, starting from 1-(tert-butoxycarbonyl)-4-piperidinone and Me anthranilate, was given. The amides I and sulfonamides such as II were tested against neuropeptide Y5 and 5-HT6 binding (data given for representative compds.). 844831-94-3P
 - 1 844831-34-3F RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 - (preparation of amides and sulfonamides as components of active combination with NPY receptor affinity and 5-HT6 receptor affinity) 844831-94-3 CAPLUS
- RN 844831-94-3 CAPLUS
 CN Benzenesulfonamide, N-[1-[2-(dimethylamino)ethyl]-1H-indol-5-yl]-2-nitro(CA INDEX NAME)

CH2-CH2-NMe2

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:136568 CAPLUS

DOCUMENT NUMBER: 142:240322

TITLE: Active substance combination comprising a compound

with NPY receptor affinity and a compound with 5-HT6

receptor affinity

INVENTOR(S): Torrens Jover, Antoni; Mas Prio, Josep; Dordal Zueras, Alberto; Codony Soler, Xavier; Merce Vidal, Ramon;

Aurelio Castrillo Perez, Jose; Frigola Constansa, Jordi; Buschmann, Helmut-Heinrich

PATENT ASSIGNEE(S): Laboratorios del Esteve S. A., Spain

SOURCE: PCT Int. Appl., 451 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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THER S	DURCE	(S):			MAR	PAT	142:	2403	22									

- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- AB The present invention relates to an active substance combination comprising at least one compound I [Rl-R4 = H, halo, alkyl, etc.; R5 = H, alkyl, (un)saturated (hetero)cycloalkyl; R6-R9 = H, alkyl, (un)saturated (hetero)cycloalkyl, etc.; A = CHRIS, CHRISCH2; R10 = H, alkyl, (un)saturated cycloalkyl, etc.; R11 = alkyl, (un)saturated cycloalkyl, etc.; RNIOR11 = (un)saturated heterocyclyl; R18 = H, alkyl, (un)saturated cycloalkyl, etc.)

with

CN

neuropeptide Y-receptor affinity, preferably neuropeptide Y5-receptor affinity, and at least one compound with 5-HT6 receptor affinity (such as II [R1 = H, alkyl, Ph, CH2PH; R2 = NR4R5, (un)saturated (hetero)cycloalkyl, etc.; R3 = H, alkyl, R4, R5 = H, alkyl; or NR4R5 = (un)saturated heterocyclyl; A = (un)substituted (hetero)aryl; n = 0-4]), a medicament comprising said active substance combination, and the use of said active substance combination for the manufacture of a medicament. Synthesis of amides I and sulfonamides such as II is described in examples. Thus, reacting 6-chloro-1-(4-piperidinyl)-1,4-dihydro-2H-3,1-benzoxazinone hydrochloride with 2-(2-chloroacetamide)-2',5-dichlorobenzophenone in the presence of K2CO3 in DMF followed by treating of the free base with HCL/EtOH afforded [61% III.RUL. The amides I and sulfonamides such as II were tested against neuropeptide Y5 and 5-HT6 binding (data given for representative compds.). 844831-94-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of amides and sulfonamides as components of active combination with NPY receptor affinity and 5-HT6 receptor affinity)

RN 844831-94-3 CAPLUS

Benzenesulfonamide, N-[1-[2-(dimethylamino)ethyl]-1H-indol-5-yl]-2-nitro-(CA INDEX NAME)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:136549 CAPLUS

DOCUMENT NUMBER: 142:240310

TITLE: Preparation of indol-5-vl sulfonamide derivatives and

their use as 5-HT6 modulators

NVENTOR(S): Merce Vidal, Ramon; Codony Soler, Xavier; Dordal

INVENTOR(S): Merce Vidal, Ramon; Codon Zueras, Alberto

PATENT ASSIGNEE(S): Laboratorios del Esteve S. A., Spain

SOURCE: PCT Int. Appl., 123 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

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PRIORITY APPLN. INFO.:
                                                                       20030730
                                               WO 2004-EP8511
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                         CASREACT 142:240310; MARPAT 142:240310
OTHER SOURCE(S):
GI
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AB Title compds. I [R1 = NR8R9 radical or (un)saturated-(un)substituted cycloaliph. radical optionally containing at least one heteroatom; R2-4,6-7 independently = H, NO2, alkoxy, CN, etc.; R5 = H or (un)saturated alkyl optionally at least monosubstituted; R8 or R9 independently = H or (un)saturated alkyl optionally at least monosubstituted with provisions; or R8 and R9 together with the bridging N atom form a (un)saturated-(un)substituted heterocyclic ring; A = (un)substituted mono or polycyclic aromatic ring; n = 0-4] and their pharmaceutically acceptable salts are prepared and disclosed

II

as 5-HT6 modulators. Thus, e.g., II, was prepared via reaction of naphthalene-2-sulfonyl chloride with 5-amino-1-(2-dimethylaminoethyl)-1Hindole. Selected data from 5-HT6 receptor binding studies revealed Ki values (nM) ranging from 1.89-112.4.

ΤТ 844831-94-3P

> RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(drug candidate; preparation of indol-5-vlsulfonamide derivs. as 5-HT6 receptor modulators)

RN 844831-94-3 CAPLUS

CN Benzenesulfonamide, N-[1-[2-(dimethylamino)ethyl]-1H-indol-5-yl]-2-nitro-(CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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TOTAL

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